

1 Supporting information for manuscript:

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3 **Perfluorinated Compounds in the Caper Fear Drainage Basin in North Carolina,**

4 **USA**

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9 Number of pages: 7

10 Number of tables: 3

11 Number of figures: 2

12

1 **Materials and Methods**

2 **Recoveries.** The recoveries were calculated by spiking PFCs into blank DI water (two
3 levels, 10 ng/L and 100 ng/L) and then passing this mixture through an SPE cartridge.
4 After elution of the PFCs from the column, the internal standards were added to the
5 eluate. The same volume of PFC-free DI water was passed through a second SPE
6 cartridge, and after elution, the same amount of the PFCs and the internal standards were
7 added to this eluate. The area ratio of the first sample was divided by that of the second to
8 give a recovery determination.

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10 **Tables**

11 Table S1. LC/MS/MS condition

12 Table S2. Mass transitions of each analyte

13 Table S3. Spearman's correlation coefficients

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15 **Figures**

16 Figure S1. LC/MS/MS chromatogram of all analytes. The chart shows total and extracted
17 ion chromatograms of the sample from the Cape Fear River at Fayetteville. Interferences
18 are separated from target analytes (red boxes).

19 Figure S2. Concentrations of PFCs and their proportion to total amounts. Charts
20 illustrates (A) stacked bar diagram of PFC concentrations (ng/L) and (B) relative
21 proportion of PFCs. Alphabetical codes stand for each river name: Cape Fear River
22 (CFR), Deep River (DR), Haw River (HR), Little River (LR), and other tributaries (OT).

23 All sampling points are ordered from the mouth to headwater of each river.

1 Table S1. LC/MS/MS condition
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HPLC	MS/MS
Instrument	Agilent 1100 (Agilent Technologies)
Column	Wakopak Fluofix-II 120E 5 µm, 3.0×100 mm (Wako Pure Chemical Industries)
Mobile phase	A: methanol, B: 2 mM ammonium acetate A:B = 0:100 (−4 to 0 min) A:B = 0:100 (0 to 1 min) A:B = 85:15 (1 to 20 min)
Flow rate	200 µL/min
Oven temperature	40°C
Injection volume	10 µL
	Instrument API 3000 (Applied Biosystems) Ionization ESI Polarity Negative Scan mode MRM Curtain gas N ₂ (9 arbitrary units, au) Nebulizer gas N ₂ (8 au) Dryer gas Zero air (8 L/min, 350°C) Ion spray −1500 V Ionization and collision cell parameters Optimized for individual analytes

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1 Table S2. Mass transitions of each analyte

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Perfluorinated Compounds	Parent Ion, m/z	Fragment Ion, m/z
C6	313	269
C7	363	319
C8	413	369
13C-PFOA	415	370
C9	463	419
C10	513	469
C11	563	519
C12	613	569
PFBS	299	80
PFHS	399	80
PFOS	499	80
18O-PFOS	503	84

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1 Table S3. Spearman's correlation coefficients

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	C12	C11	C10	C9	C8	C7	C6	PFOS	PFHS	PFBS
C12	1.0000 N = 15	0.9385** 14	0.2879 14	0.6214* 15	0.4021 15	0.7071** 15	0.6953** 14	-0.0286 15	0.0429 15	0.5238 8
C11		1.0000 34	0.7438** 34	0.7894** 34	0.6281** 34	0.7437** 32	0.6913** 29	0.1499 34	-0.0934 31	0.3170 18
C10			1.0000 49	0.8656** 49	0.7860** 49	0.7493** 39	0.6185** 32	0.0592 49	-0.3663* 42	0.3930* 26
C9				1.0000 59	0.8292** 59	0.8121** 43	0.7652** 35	0.3203* 59	-0.1190 51	0.5401** 30
C8					1.0000 65	0.7821** 44	0.7250** 35	0.5344** 65	-0.0439 51	0.6138** 30
C7						1.0000 44	0.7677** 35	-0.1891 44	-0.4014** 42	0.6195** 27
C6							1.0000 35	-0.1052 35	-0.4022* 35	0.5210* 21
PFOS								1.0000 77	0.5876** 58	0.4006* 31
PFHS									1.0000 58	0.2467 31

*: p < 0.05, **: p < 0.01, Shaded values show significant correlations.

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Figure S1

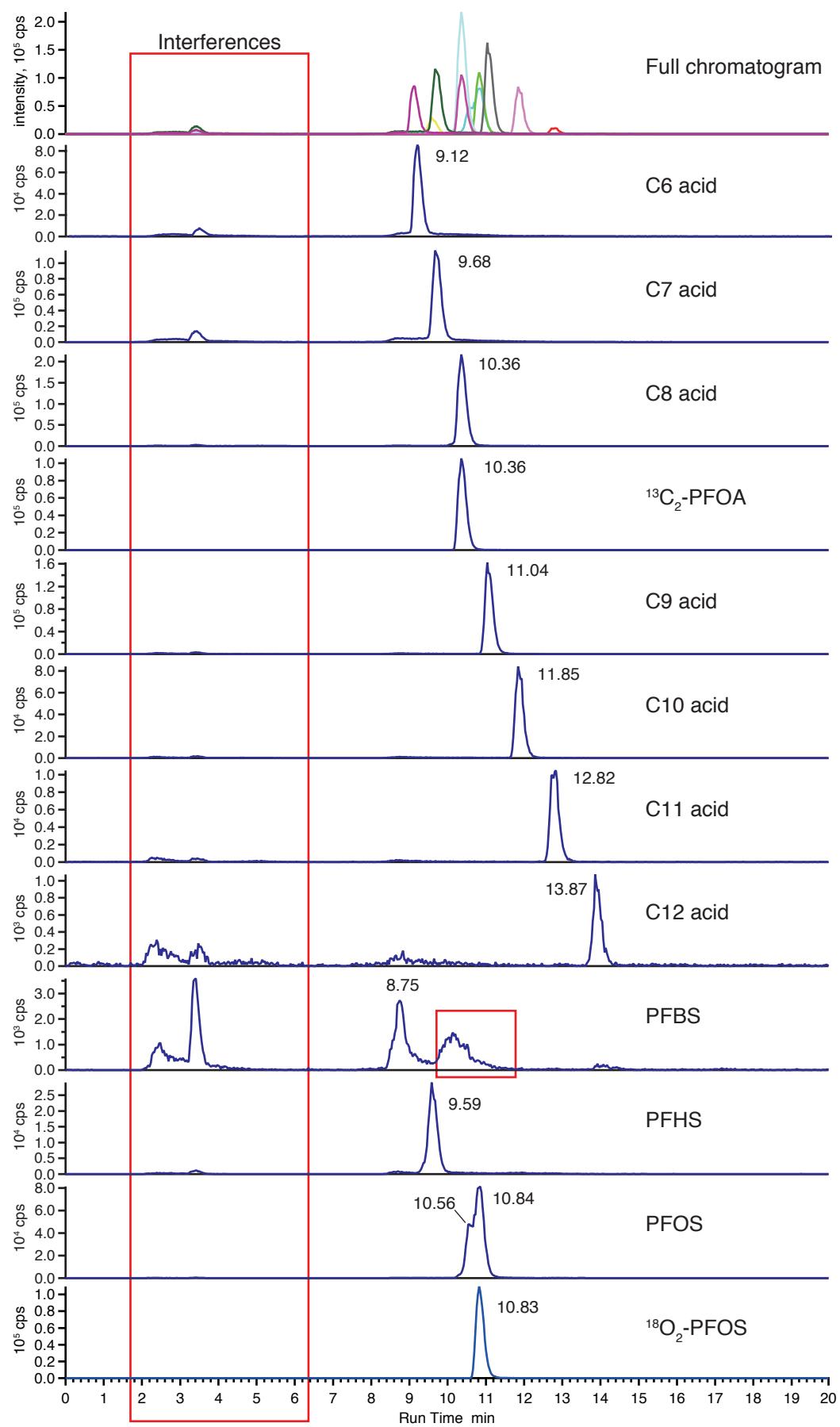
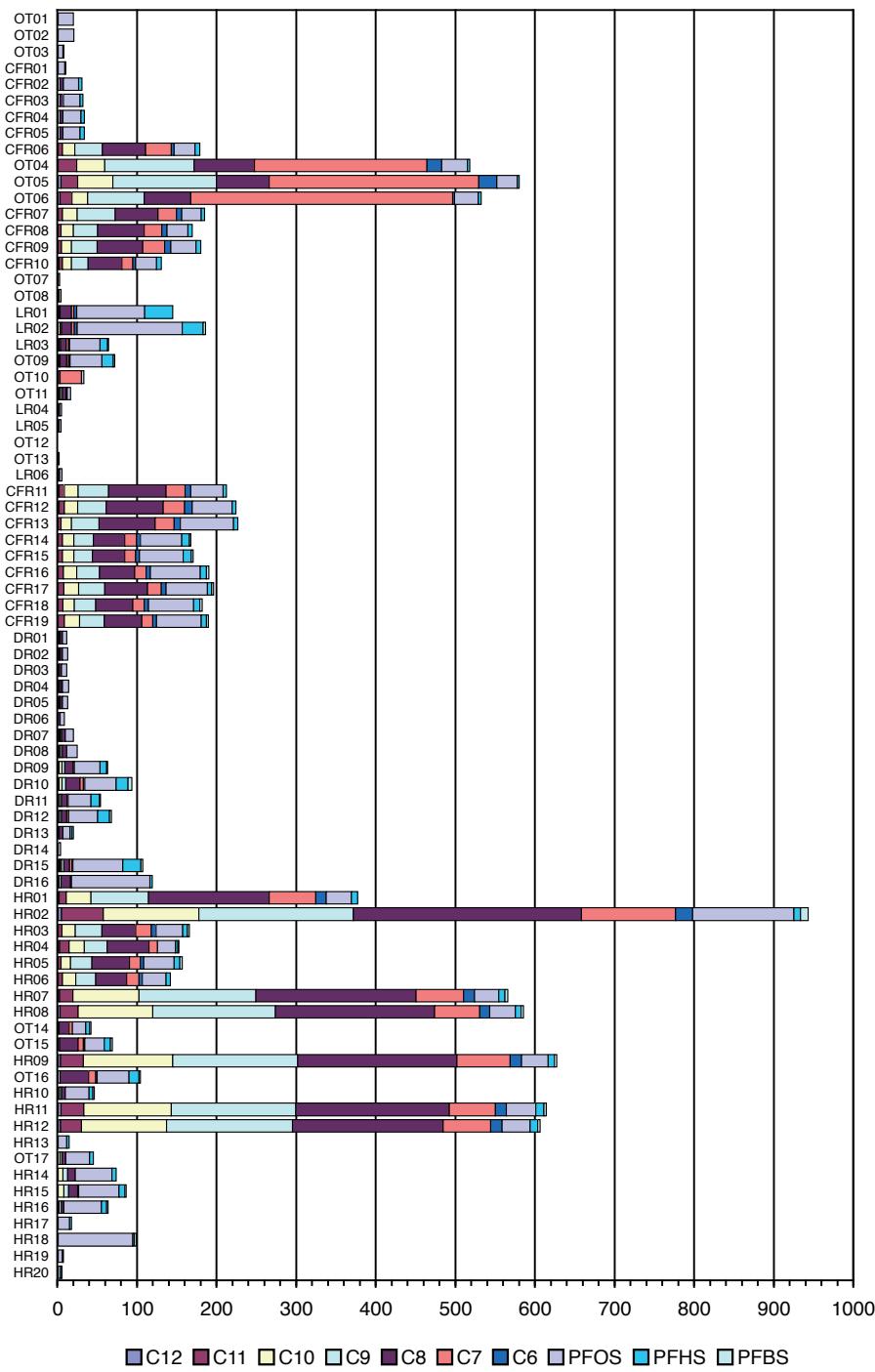


Figure S2

(A)



(B)

